

## Supplementary Material

### 1 DATA AVAILABILITY

The datasets generated and analyzed in this study, along with codes, can be found in the Antibiofilm repository at

[github.com/davidanastasiu/antibiofilm](https://github.com/davidanastasiu/antibiofilm).

### 2 DATASET STATISTICS

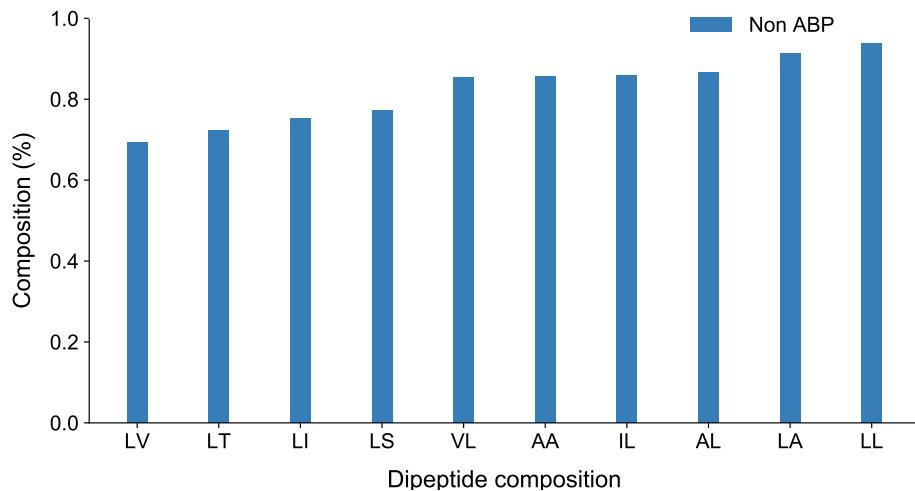
Table S1 presents the number of peptides for training, validation and out-of-sample test sets for both the positive and negative datasets. The table also contains details of the dataset used for training and evaluating the regression models.

**Table S1.** Dataset Distribution of Our Machine Learning Models

Dataset	Type	Training	Validation	Out-of-Sample Test
Classification	Positive	175	19	48
	Negative	1741	194	485
MBIC Classification	$\leq 64\mu\text{M}$	128	32	N/A
	$> 64\mu\text{M}$	14	4	N/A
MBIC Regression	$\leq 64\mu\text{M}$	128	32	N/A
	$\leq 64\mu\text{M}$	33	9	N/A
Candidate		135015		

### 3 CHARACTERIZATION OF PEPTIDES

Figure S1 presents the ten dipeptides with the highest composition percentage from the negative dataset. Interestingly, most of the dipeptides in the top ten set contain leucine, a non-polar amino acid.



**Figure S1.** Dipeptide composition of the negative dataset; all the dipeptides contain the non-polar amino acid leucine;

#### 4 PERFORMANCE OF MACHINE LEARNING MODELS

Table S2 presents results from our evaluation of different machine learning models based on individual features while Table S3 displays the performance of different models when we combine two features together. Finally, Table S4 showcases the performance of our models when we combine more than two features. Our best performing model combines the AAC, DPC, CTD and Motif features.

**Table S2.** Performance Evaluation of Different Machine Learning Techniques with Individual Features

Feature	Model	Sensitivity	Specificity	Accuracy	F1 Score	MCC
AAC	SVM	72.91	99.79	97.37	83.33	82.93
	RF	68.75	100	97.18	81.48	81.66
	XGBoost	75.11	99.38	97.18	82.75	81.76
DPC	SVM	85.41	98.35	97.17	84.35	82.99
	RF	72.91	99.17	96.81	80.45	79.24
	XGBoost	79.16	98.76	96.99	82.60	81.06
CTD	SVM	83.33	99.38	97.93	86.94	87.91
	RF	70.83	99.79	97.18	81.92	81.62
	XGBoost	85.41	98.96	97.74	87.23	86.02

**Table S3.** Performance Evaluation of Different Machine Learning Techniques with a Combination of Two Features

Features	Model	Sensitivity	Specificity	Accuracy	F1 Score	MCC
AAC & DPC	SVM	81.25	98.96	97.33	84.78	83.33
	RF	77.08	99.79	97.74	86.08	85.52
	XGBoost	81.25	99.38	97.74	86.66	85.76
DPC & CTD	SVM	77.08	99.79	97.74	86.04	85.52
	RF	70.83	100	97.37	82.92	82.97
	XGBoost	79.16	99.17	97.37	84.44	83.23
CTD & AAC	SVM	85.41	99.17	97.93	88.17	87.09
	RF	72.91	100	97.56	84.33	84.26
	XGBoost	79.16	99.58	97.74	86.36	85.56

**Table S4.** Performance Evaluation of Different Machine Learning Techniques with a Combination of Three or More Features

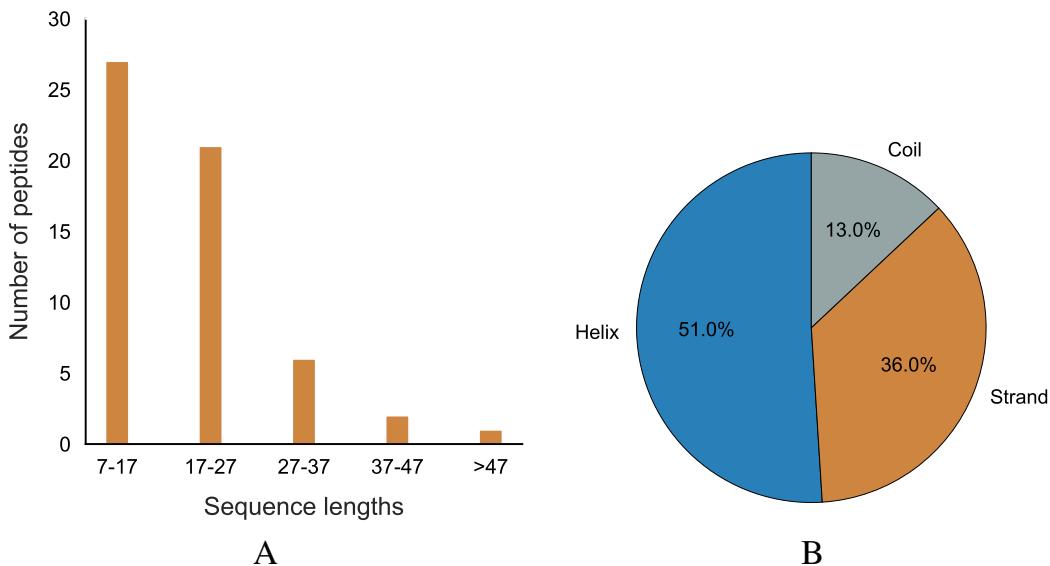
Features	Model	Sensitivity	Specificity	Accuracy	F1 Score	MCC
AAC & DPC & CTD	SVM (c=100, gamma=0.01)	85.41	98.96	97.94	88.42	87.29
	RF (n-estimator=100)	70.83	100	97.37	82.92	82.97
	XGBoost (n-estimator=100, gamma=0.5)	81.25	99.58	97.93	87.64	86.84
AAC & DPC & CTD & motif	SVM (c=150, gamma=0.05, Motif=ALL)	<b>85.48</b>	<b>99.79</b>	<b>98.49</b>	<b>91.11</b>	<b>90.53</b>
	RF (with Motif=BETTS-RUSSELL)	72.91	100	97.56	84.33	84.26
	XGBoost (with Motif=BETTS-RUSSELL)	85.41	99.38	98.12	89.13	88.20

**Table S5.** Performance Comparison of Our Method with the Dataset from [Gupta et al. \(2016\)](#)

Validation dataset performance	Specificity	Sensitivity	Accuracy	F1 Score	MCC
Reported in <a href="#">Gupta et al. (2016)</a>	97.75	91.67	97.19	N/A	0.84
Achieved with our model	<b>99.71</b>	86.11	<b>98.46</b>	<b>91.17</b>	<b>0.90</b>

## 5 CHARACTERIZATION OF PEPTIDES FROM THE MBEC DATASET

We present the characteristics of the 57 peptides that were selected for training the regression model responsible for predicting the MBEC value of a candidate antibiofilm peptide.



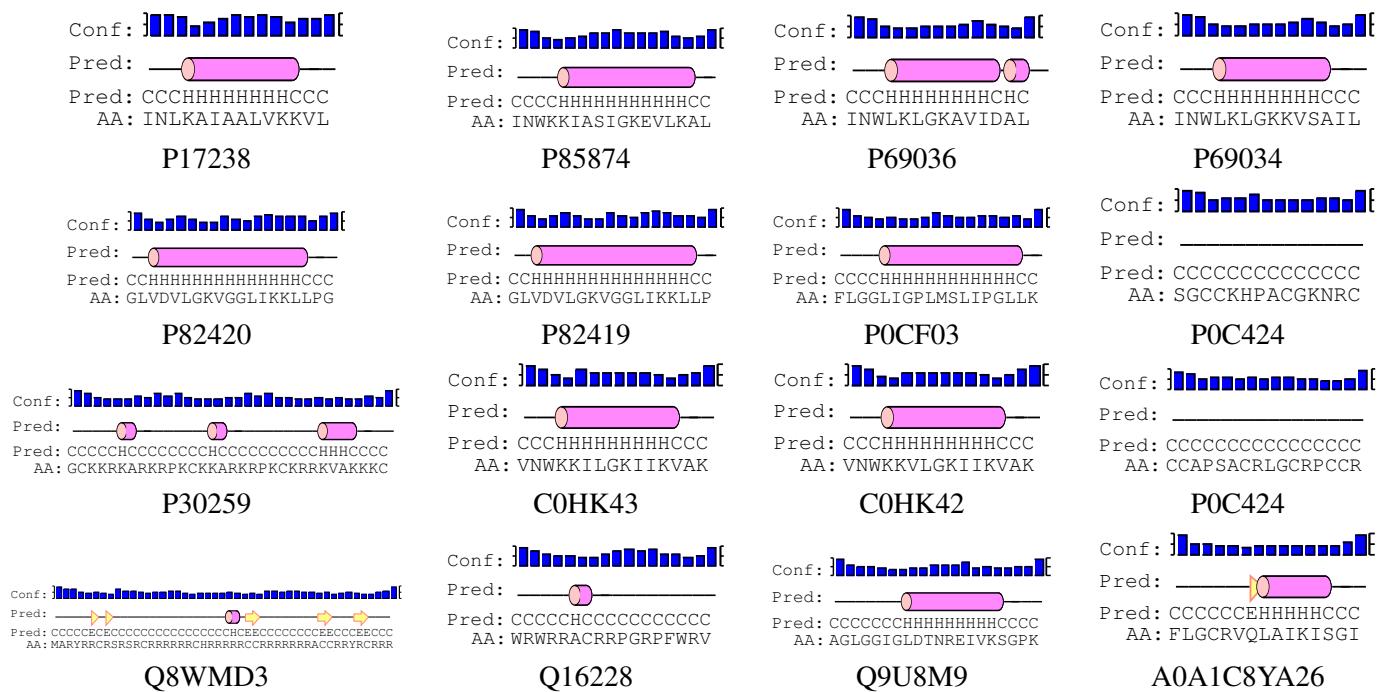
**Figure S2. Performance and characteristics of peptides with MBIC/MBEC values;** (A) Number of peptides with MBEC values in different sequence ranges; (B) Percentage of helices, strands and coils in secondary structure for peptides with MBEC values;

## 6 NEWLY FOUND ANTIBIOFILM PEPTIDES

### 6.1 Visualization

We have evaluated the 2D structures of the peptides using PEP2D server [Singh et al. \(2019\)](#).

We further evaluated the structure of the peptides with probable antibiofilm activity. We evaluated helical wheel structure (Figure S5) for the peptides which showed higher percentage of helices in secondary structure evaluation.



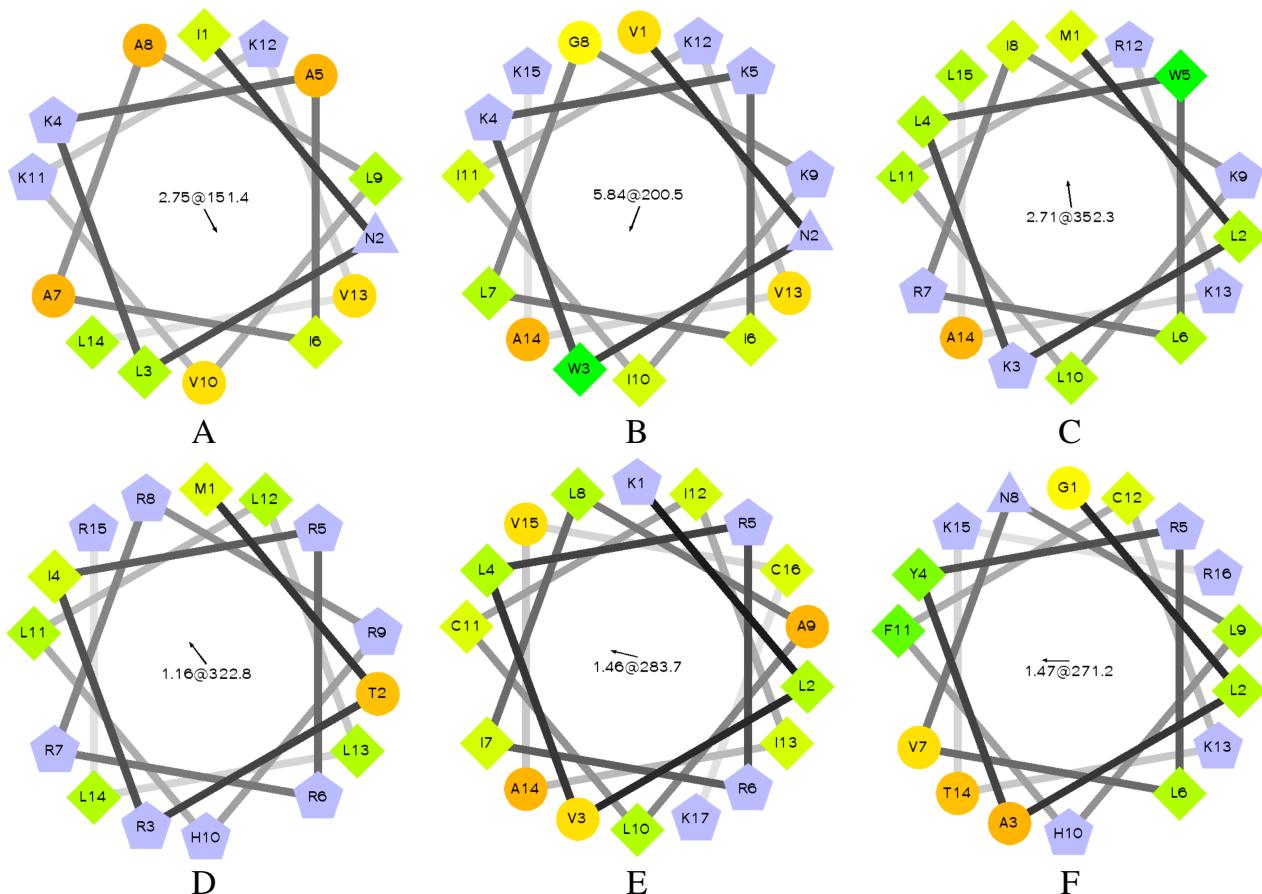
**Figure S3. Predicted 2D structures of previously characterized peptides with potential antibiofilm activity.**

The 2D structures were evaluated using the PEP2D server. The pink cylinders represent helix, yellow arrows represent sheet, and the black line is coil.



**Figure S4.** Predicted 2D structures of previously characterized peptides with potential antibiofilm activity.

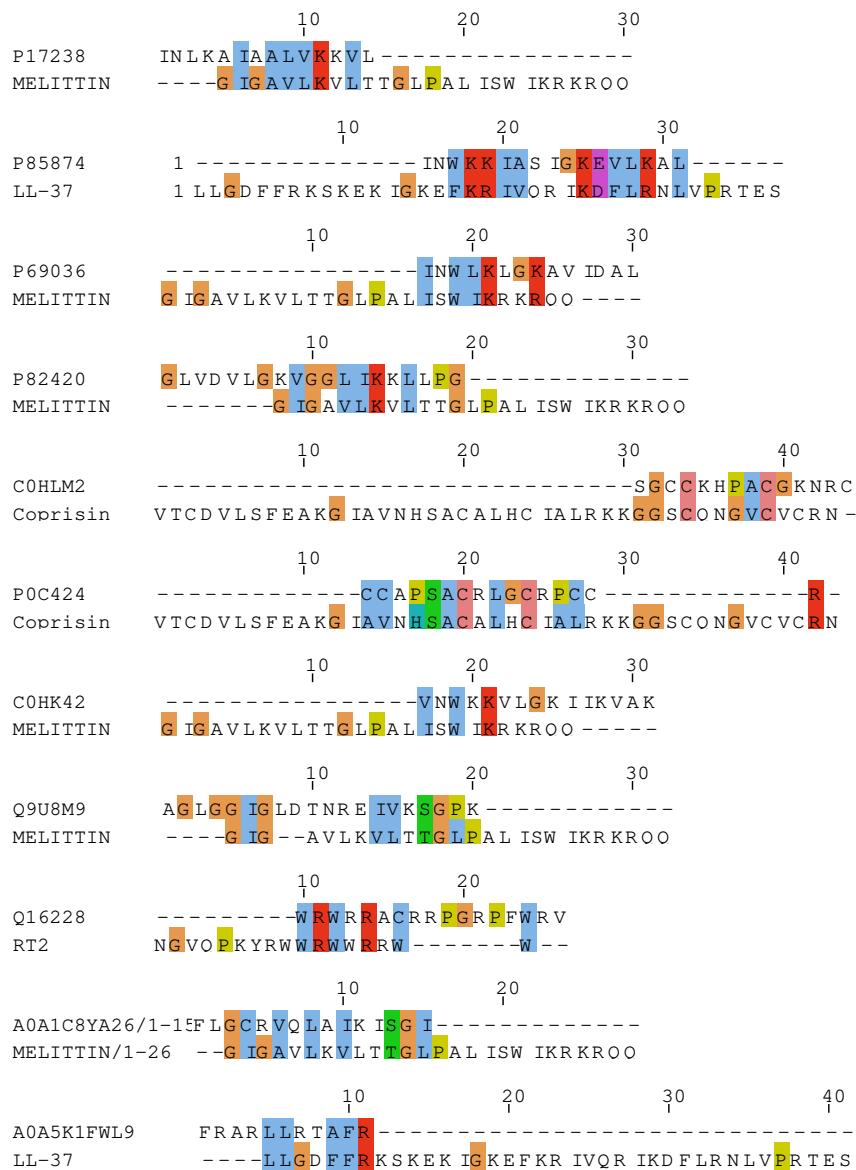
The 2D structures were evaluated using the PEP2D server. The pink cylinders represent helix, yellow arrows represent sheet, and the black line is coil



**Figure S5. The helical wheel structures of a few newly found antibiofilm peptides;** (A) P17238, Mastoparan; (B) C0HK43, Lasioglossin; Rest of the peptide marked as 'uncharacterized protein' (C) A0A2P2Q2Y8, (D) A0A0A9U210, (E) E9JAR4, (F) A0A3Q7GQZ6. Here, hydrophilic amino acids are shown in circles, hydrophobic as diamonds. Negatively charged amino acids are triangles, and positively charged are pentagons. The hydrophobic amino acids are green, and the green shade decreases to yellow as per decreasing hydrophobicity. Hydrophilic amino acids are in red and the amount of red decreases as per decreasing hydrophilicity. The highly charged amino acids are in light blue and non-polar amino acids are in dark red. The numbers indicate the hydrophobic moment and the direction of the moment. The wheel structures were obtained using the software created by Don Armstrong and Raphael Zidovetzki, version 1.4, 2009-10-20 [Schiffer and Edmundson \(1967\)](#); [Armstrong and Zidovetzki \(2009\)](#).

## 6.2 Alignment

We also analyzed a few newly found antibiofilm peptides against some well known antibiofilm peptides which already have an eradication effect on preformed biofilm. For example, we aligned human cathelicidin, LL-37, against the set of Mastoparan-like peptides from our list. The alignment was done using the Clustal default webservice [Madeira et al. \(2019\)](#). The alignment is displayed in Figure S6 using Jalview V2 [Waterhouse et al. \(2009\)](#).



**Figure S6. Pairwise sequence alignment of peptide hits with their closely matching known antibiofilm peptide. The default colour scheme used as per ClustalX**

Colorcode – blue: residue A, I, L, M, F, W, V, C; red: residue K, R; green: residue N, Q, S, T; magenta: E, D; yellow: residue P.

### 6.3 Peptide List

The list of probable antibiofilm peptides from our pipeline are listed in Tables S6–S13. The tables contain peptide sequences and predicted MBEC values. We grouped the peptides in several MBIC value ranges.

**Table S6.** Newly Predicted Antibiofilm Peptides with MBIC Range 1–8 ( $\mu\text{M}$ ) from the DRAMP database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
DRAMP04642	GIGKFLHSAGKFGKAFIGEIMKS	Synthetic	1.510
DRAMP02364	GFWGKLFKLGLHGIGLLHLHL	Mammals	1.617
DRAMP04663	AKRLKKLAKKIWKWL	Sheep	1.617
DRAMP01423	GLLSGILGAGKHTVCGLSGLR	Synthetic	3.071
DRAMP18605	VNWKKILAKIIKVVK	Synthetic	3.597
DRAMP18607	VNWKKILPKIICKVVK	Synthetic	4.332
DRAMP03983	KWKLFKKIPKFLHLA	Synthetic	4.332
DRAMP03862	RLRRIVVIRVRR	Frog	6.605
DRAMP01310	FLGLLPSIVSGAVSLVKKL	Synthetic	7.090
DRAMP04187	KWLKKLLKKLL	Synthetic	8.957
DRAMP03974	WKKIPKFLHLAKKF	Fish	9.853
DRAMP18601	VNWKKILAKIIKVAK	Synthetic	11.312
DRAMP18602	VNWKKILKKIIKVAK	Synthetic	11.854
DRAMP18603	VNWKKILPKIICKVAK	Synthetic	13.681
DRAMP03981	KWKLFKKIPKFLHLAK	Synthetic	20.981
DRAMP03850	FALALKALKALKLKKALKKAL	Scorpion	22.396
DRAMP04002	ILGKILKGKIKLFL	Xenopus muelleri	22.471
DRAMP18560	IWRIFRRIFRIF	Synthetic	22.608
DRAMP03859	RLARIVVIRWAR	Synthetic	22.632
DRAMP03880	RRIIIRWRRI	Synthetic	22.668
DRAMP04318	IKWKKLLRAAKRIL	Synthetic	22.671
DRAMP18642	KWRWIW	Bacteria	22.674
DRAMP04297	LKALKLAKKLKKLA	Synthetic	22.677
DRAMP04215	RRLFRRILRWL	Synthetic	22.677
DRAMP18514	KKLALHALKKWLHALKKLAHLALKK	Synthetic-De Novo	22.679
DRAMP04384	KIASIGKEVLKAL	Synthetic	22.679
DRAMP03702	LFGLIPSLIGGLVSAFK	Synthetic	22.679
DRAMP02910	LRRIIRKIIHIIKK	Synthetic	22.679
DRAMP02911	IRRIIRKIIHIIKK	Synthetic	22.725
DRAMP01621	IIGPVLMVGVSALGGLKKI	Synthetic	22.837
DRAMP01626	IIGPVGLVGVSALGGLKKI	Synthetic	24.947
DRAMP04125	SGKLWWRRKK	Frog	25.316
DRAMP03975	KWFKKIPKFLHLLKKF	<i>Bombina variegata</i>	25.316
DRAMP03973	WFKKIPKFLHLAKKF	Synthetic	25.568
DRAMP03979	KWKLFKKIPKFLHLAKK	Orange-legged leaf frog	25.616
DRAMP01807	FLPLVLGALSGILPKIL	Synthetic	29.105
DRAMP03977	WKKIPKFLHLLKKF	Synthetic	29.774
DRAMP03976	WFKKIPKFLHLLKKF	Synthetic	36.868
DRAMP18619	RKLRLRKRIAHKVKKY	Synthetic	60.154

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**Table S7.** Newly Predicted Antibiofilm Peptides with MBIC Range 8–16 ( $\mu\text{M}$ ) from the DRAMP Database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
DRAMP02474	KFFRKLLKSVKKRAK	Spider	2.397
DRAMP18600	NVWKKILGKIIKVAK	Synthetic	2.462
DRAMP18568	VSWKKS LGKIIKVVK	Synthetic	3.071
DRAMP18596	NVWKVVLGKIIKVAK	Synthetic	3.071
DRAMP04228	GRF RRLGRKF KKLFKKYGP	Synthetic	3.071
DRAMP03972	KWF K KIPKFLHLAKKF	Scorpion	3.236
DRAMP02963	GRF RRLRK KTRKL KIGKV	Synthetic	4.011
DRAMP01126	ILGPV ISKIGGV LGG LKL N	Synthetic	4.332
DRAMP03570	LLGDFFRKSKE KIGKEF K RIVQR	Bovine	4.719
DRAMP03967	KWKL FK KIPKFLHLAKKF	Synthetic	4.953
DRAMP03969	KWKL FK KIS KFLHLAKKF	Synthetic	4.953
DRAMP03970	WKL FK KIPKFLHLAKKF	Synthetic	6.610
DRAMP03971	FKL FK KIPKFLHLAKKF	Synthetic	10.699
DRAMP18563	KSL RR VWR SWR	Synthetic	10.791
DRAMP03826	KNL RRI IRK II HII KYG	<i>Odorrana grahami</i> (Frog)	15.718
DRAMP04310	ELAKKALKALKALKSAR	Synthetic	16.091
DRAMP04311	ELAKKAL RALKALKSAK	Pig	19.720
DRAMP03227	GLFGK LKK FGRKA ISYAVKKARGKH	Synthetic	19.996
DRAMP03980	KWKL FK KIPKFLHLAKKF	Toad	21.695
DRAMP03923	KWKL FK KIGIGAVLK VLT	Synthetic	22.608
DRAMP04260	LALL KVLL R KIKK AL	Synthetic	22.645
DRAMP18562	KSL VRR WRS RW	Synthetic	22.645
DRAMP18597	VNW KVL A KII KVAK	Synthetic	22.659
DRAMP18598	VNW KVL KII KVAK	Synthetic	22.659
DRAMP18599	VNW KVL P KII KVAK	Synthetic	22.668
DRAMP03963	KWKL FK KIK FLHS AKKF	Synthetic	22.671
DRAMP03968	KWKL FK KIL KFLHLAKKF	Synthetic	22.676
DRAMP03984	KWKL FK KIP LAKKF	Synthetic	22.679
DRAMP18570	VNR K KIL GKS I KVVK	Synthetic	22.679
DRAMP18502	WKS YVRR WR	Synthetic	22.679
DRAMP04018	ALYKK FK KLL KSL KRL G	Bacteria	22.679
DRAMP04003	ILG KI W KIK KLF	Synthetic	22.679
DRAMP04376	INWL KLG KKI ISAL	Synthetic	22.705
DRAMP18507	FSGGN CRGF RRC FCTK	Synthetic	22.725
DRAMP04614	AVNIP FKVH FRCK SIFC	Synthetic	22.837
DRAMP03865	RWW KI W V RWW R	Synthetic	22.837
DRAMP18567	VNW KIL GKS I KVSK	Synthetic	23.595

**Table S8.** Newly Predicted Antibiofilm Peptides with MBIC Range 8–16  $\mu\text{M}$  from the DRAMP Database (Cont.)

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
DRAMP04664	AKRLKKLAKKIWKWK	Human	24.958
DRAMP04051	RICRIVVIRCIR	Human	25.040
DRAMP03978	KWKLFFKKIPFLHLAKKF	Synthetic	25.219
DRAMP03925	KWKLFFKGAVLKVLT	Synthetic	25.595
DRAMP03768	ILSAIWSGIKS	Synthetic	25.595
DRAMP03858	RLARIVKIRVAR	Synthetic	25.595
DRAMP03982	KWKLFFKKIPHLAKKF	Synthetic	28.344
DRAMP18564	KWLRRVWRWWWR	Snake	35.077
DRAMP18565	KRLRRVWRWRWR	Synthetic	39.599
DRAMP03964	KWKLFFKKIPKFLHSACKF	Synthetic	39.927
DRAMP03924	KWKLFFKGIGAVLKV	Synthetic	44.372
DRAMP03575	FKRIVQRIKDFLR	AnTomato	48.038
DRAMP02872	GRFKRFRKKFKLFFKKLKS	Synthetic	50.828
DRAMP18501	WKSYVRRWRS	Synthetic	53.153
DRAMP03829	GLKLLGKLLKKLGKLLLK	Synthetic	54.066
DRAMP18499	WKSYVRRWRSR	Synthetic	63.560

**Table S9.** Newly Predicted Antibiofilm Peptides with MBIC Range 16–32 ( $\mu\text{M}$ ) from the DRAMP Database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
DRAMP03777	IWSAIWSGIKGLL	<i>Urodacus yaschenkoi</i> (scorpion)	35.514
DRAMP04390	INWKKGKEVLKAL	Synthetic	22.679
DRAMP03966	KLKLFFKKIGIGKFLHSACKF	Synthetic	7.220
DRAMP02914	RICRIIFLRVCR	Sheep	14.287
DRAMP04377	INWLKLGKKLLSAL	Synthetic	22.679
DRAMP04113	KWKSFIKKLASKFLHSACKF	Synthetic	22.680
DRAMP04115	KWKSFIKKLTKKFLHSACKF	Synthetic	45.279
DRAMP04127	RGKRWWRKK	Synthetic	49.900
DRAMP04054	RLCRIIVWVIRVCR	Synthetic	47.017
DRAMP18401	ILSAIWSGIKGLL	Scorpion	35.514
DRAMP03965	KAKLFKKIGIGKFLHSACKF	Synthetic	5.068
DRAMP04102	KWKSFIKKLTSKFLHLAKKF	Synthetic	25.740
DRAMP04103	KWKSFIKKLTSKFLHSACKF	Synthetic	45.279
DRAMP04104	KFKSFIIKKLTSKFLHSACKF	Synthetic	45.279
DRAMP04106	KWKSFKKKLTSKFLHSACKF	Synthetic	45.279
DRAMP04119	KWKSFIKKLTSKFLHSKKKF	Synthetic	45.279
DRAMP04112	KWKSFIKKLTSKFLHSACKF	Synthetic	22.380
DRAMP18723	KWKLFFKI	Moth	48.126
DRAMP18566	VNWKKSLGKSIKVVK	Synthetic	4.953
DRAMP01134	ILGPVIKTIGGVLGGLLN	Toad	19.866

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**Table S10.** Newly Predicted Antibiofilm Peptides with MBIC Range >32 ( $\mu\text{M}$ ) from the DRAMP Database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
DRAMP04343	IGKLFKRIVKRILKFLRKL	Synthetic	35.719
DRAMP04126	SGKRWWRKK	Synthetic	49.900
DRAMP04339	IGKKFKRIVQRIKKFLRKL	Synthetic	3.556
DRAMP04340	IGKKFKRIVKRIKKFLRKL	Synthetic	3.556
DRAMP04345	IGKKWKRIVKRIKKFLRKL	Synthetic	3.556
DRAMP04346	IGKKFKRIVKRIKKWLRKL	Synthetic	3.556
DRAMP18614	VRRFAWWAFLRR	Synthetic	22.940
DRAMP03876	RRWWWWRWRRW	Synthetic	49.900
DRAMP03877	KKWWWKWKKW	Synthetic	49.900
DRAMP03878	RRWWWRWRRW	Synthetic	49.900
DRAMP03879	RRFFFRRFRF	Synthetic	49.900
DRAMP18457	KRWWKWWRRC	Synthetic	15.828
DRAMP18508	KFAKKFKWFAKAAFKFFKK	Synthetic	49.900
DRAMP18643	KWWWRW	Synthetic	49.900
DRAMP04001	ILGKIWKGIKSLF	Synthetic	7.590
DRAMP04069	CFKFKFKFGSGFKFKFC	Synthetic	22.791
DRAMP04070	CWKWKWKWGSGWKWKWC	Synthetic	22.791
DRAMP03869	RRWVIWRR	Synthetic	40.529
DRAMP18558	FIKRIARLLRKIF	Synthetic	34.455

**Table S11.** Newly Predicted Antibiofilm Peptides with MBIC Range 1–8 ( $\mu\text{M}$ ) from the UniProt database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
sp—P0CF03—	FLGGGLGPLMSLIPGLLK	Ant	19.723
tr—A0A5K1B3V0—	VIRIGCKWKRTA	<i>Nymphaea colorata</i> (plant)	6.260
tr—A0A0E9SZ00—	MCTRWRVLLTCVRRR	<i>Anguilla anguilla</i> (eel)	28.711
tr—A0A2P2N8A3—	MGGKSDFRFCHVKKKVL	<i>Rhizophora mucronata</i> (plant)	11.138
tr—A0A0A9M1Q7—	MGRKFKWKLWT	<i>Arundo donax</i> (plant)	14.310
sp—C0HK43—	VNWKKILGKIIKVAK	<i>Lasioglossum laticeps</i> (bee)	3.071
tr—A0A0A9U210—	MTRIRRRLHLLLLR	<i>Arundo donax</i> (plant)	22.612
sp—P17236—	FLPLILGKLVKGLL	Oriental hornet	36.241
tr—A0A2P2Q2Y8—	MLKLWLRIKLLRKAL	<i>Rhizophora mucronata</i> (plant)	35.601
tr—A0A5K1FWL9—	FRARLLRTAFR	<i>Nymphaea colorata</i> (plant)	22.722
sp—P82419—	GLVDVLGVGGGLIKKLLP	Ant	28.502
sp—C0HLD5—	FLSLIPKIAGGIASLVKNL	Frog	23.319
sp—P82420—	GLVDVLGVGGGLIKKLLPG	Ant	27.711
tr—E4Z311—	IKGILLRKIIKVR	<i>Oikopleura dioica</i> (tunicate)	35.514

**Table S12.** Newly Predicted Antibiofilm Peptides with MBIC Range 8–16 ( $\mu\text{M}$ ) from the UniProt database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
tr—A0A3D5SU75—	PCPCGSGKKYKHCHGKLS	<i>Rhodocyclaceae bacterium</i>	1.854
sp—P0C424—	CCAPSACRLGCRPCCR	<i>Conus marmoreus</i> (marble cone)	2.968
tr—A0A5K1BN05—	LGC GHGLPGIFACLK	<i>Nymphaea colorata</i> (plant)	3.071
tr—A0A5K1DCQ4—	LGC GHGLPGIYACLK	<i>Nymphaea colorata</i> (plant)	3.071
sp—C0HK42—	VNWKKVLGKIIKVAK	<i>Lasioglossum laticeps</i> (bee)	3.071
sp—P30259—	GCKKRKARKRPKCKKARKRPKCKRRKVAKKKC	Catshark	4.290
sp—P14215—	RRWCFRVCYRGFCYRKCR	Atlantic horseshoe crab	6.030
sp—P14216—	RRWCFRVCYKGFCYRKCR	Atlantic horseshoe crab	6.030
tr—A0A0G3VIX2—	AVPSWRIKSWNR	Bacteria	7.090
tr—E9I8P2—	MLKKFLGKSGRRILR	<i>Solenopsis invicta</i> (ant)	8.156
sp—P69135—	KWCFCRV CYRGICYRRCR	Asian horseshoe crab	18.171
sp—Q8WMD3—	MARYRRCRSRSRCRRRRCHRRRRCCRRRRRA CCRYRCRR	Bat	21.567
tr—A0A0D3HK27—	MFGGSGPLKL	<i>Oryza barthii</i> (plant)	22.009
tr—A0A1C8YA26—	FLGCRVQLAIKISGI	<i>Triticum aestivum x Aegilops sharonensis</i> (plant)	22.359
tr—A0A3Q7GQZ6—	GLAYRLVNLHFCKTKR	<i>Solanum lycopersicum</i> (tomato)	22.657
tr—A0A0K1NW40—	KAIALALGKGCK	<i>Lycium cestroides</i> (plants)	22.679
sp—P0C022—	INLLKIAKGIKSL	Wasp	22.679
sp—P85874—	INWKKIASIGKEVLKAL	Wasp	22.679
sp—P69034—	INWLKLGGKKVSAIL	Wasp	22.679
sp—P69036—	INWLKLGGKAVIDAL	Wasp	22.679
sp—P85443—	GLLDFLKAAGKGLVTNL	Frog	22.691
tr—A0A5K0UXG7—	ALLKSKPKLLRSGL	<i>Nymphaea colorata</i> (plant)	22.694
tr—E9JAR4—	KLVLRRILALCIIAVCK	<i>Solenopsis invicta</i> (ant)	22.924
sp—P82282—	IIGPVLMGVGSALGGLKKIG	Toad	23.278
sp—P82285—	IIGPVGLGVGSALGGLKKIG	Toad	23.278
sp—P85982—	IFGAILPLALGALKNLIK	Frog	23.712
LFB0040	FKCRRWAWRMKKLGA	Synthetic	25.902
sp—P0C1R0—	ILGTILGLLKS	Wasp	32.702
tr—A0A5K0UVL7—	ILLIKVGCCKIK	<i>Nymphaea colorata</i> (plant)	38.404
LFB0017	FKCRRWQWR	Lactoferrin, source: cow	38.492
sp—C0HLM2—	SGCCKHPACGKNRC	Alpha-conotoxin, source: conus purpurascens	39.130
tr—A0A0K0LBU6—	GGYCGGAFRQRCICYRK	<i>Androctonus bicolor</i> (scorpion)	46.616
tr—A0A5K1F988—	EKF KIHKGKRW	<i>Nymphaea colorata</i> (plant)	46.812
tr—I7DAN2—	KKSGKIKSAYKR	<i>Rhea americana</i> (bird)	50.828
tr—S7IKV4—	SGLFCKGCSKL	<i>Chlamydia psittaci</i> (bacteria)	60.154
tr—Q16228—	WRWRRACRRPGRPFWRV	Human	61.163

**Table S13.** Newly Predicted Antibiofilm Peptides with MBIC Range 16–32 ( $\mu\text{M}$ ) from the UniProt database

Name	Seq	Source	Predicted MBEC ( $\mu\text{M}$ )
sp—P0C005—	GLLKRIKTLL	Wasp	22.679
sp—P17238—	INLKAIAALVKV	Hornet	22.679
tr—Q9U8M9—	AGLGGIGLDTNREIVKSGPK	<i>Scaptomyza graminum</i> (insect)	20.318

## 7 DATASET

### 7.1 Positive Dataset

The details of our positive dataset, including the peptide sequence and its length, are given in Tables S14–S18.

**Table S14.** Peptide List for our Positive Dataset

Name	Seq	Seq Length
BREVININ-1GHA	FLGAVLKVAGKLVPAIAICKISKKC	24
DERMASEPTIN-AC4	SLWGKLKEMAAAAGKAALNAVGLVNQ	27
RPDEF1ALPHA	GFGCPNDYSCSNHCRDSIGCRGGYCKYHVICTCYGCKRRIQE	44
KASSINIATUERIN-3	FIQHLIPLIPHAIQGIKDIF	20
AGELAIA-MP	INWLKLGKAIDAL	14
CCL20	SNFDCCCLGYTDRILHPKFIVGFTRQLANECDINAIIFFHTKKKLSVCANPKQTWVKYIVRLLS KKVKNM	69
CHICKEN	RFGFRFLRKIRRFRPKVTITIQQSARFG	27
CITROPIN	GLFDVIKKVASVIGGL	16
COLISTIN	KTKKKLLKKKT	10
CON10	FWSFLVKAASKILPSLIGGGDDNKSSS	27
COPRISIN	VTCDVDLSFEAKGIAVNHSACALHCIALRKGGSCQNGVCVCRN	43
DATUCIN	TFPKCAPTRPPGPKPCDINNFKSKFWHIWRA	31
DERMASEPTIN-PH	ALWKEVLKNAGKAALNEINNLV	22
DERMASEPTIN-PT9	GLWSKIKDAAKTAGKAALGFVNEMV	25
DHV4R	KRLFKKKLFSLRKY	14
ENTEROCIN	LGSCVANKIKDEFFAMISISAIVKAAQKKAWKELAVTVLRFAKANGLKTNAIIVAGQLALWAV QCGLS	68
ESCULENTIN	GIFSKLAGKKIKNLLISGLKG	21
GL13K	GKIIKKLKLASKLKL	13
GRAMICIDIN	VKLFPVKLFP	10
HS02	KWAVRIIRKFIKGFI	16
HUMAN defensin	GIINTLQKYYCRVRRGGRCAVLSCLPKEEIQIGKCSTRGRKCCRRKK	45
HYICIN	NKGCSACAIGAACLAQGPPIPDEVAGITGTGFIAS	35
INDOLICIDIN	ILPWKPWPWWPWRR	13
JAPONICIN-2LF	FIVPSIFLLKKAFCIALKKC	20
LL-37	LLGDFFRKSKEKIGKEFKRIVQRIKDFLRNLVPRTES	37
MP-C	LNLKALLAVAKKIL	14
MORONECIDIN-	FFRNLWKGAKAAFRAFGHAAWRA	22
MYXINIDIN	GIHDILKYGKPS	12
NA-CATH	GLLSGILGAGKKIVF	15
NISIN	ITISLCTPGCKTGALMGCNMKTATCHCSIHVSK	34
PARACENTRIN	EVASFDFDKSKLK	11
PHYLLOSEPTIN-1	FLSLIPHIVSGVSIAKHF	19
PHYLLOSEPTIN-CO	FLSMIPKIAGGIASLVKNL	19
PHYLLOSEPTIN-PHA	FLSLIPAAISAVSALANHF	19
PLEUROCIDIN	GWGSFFKKAHVGVKHVGKAALTHYL	25
POLYBIA-MP-II	INWLKLGKMKVIDAL	14
POLYMYXIN	KTKKKFLKKKT	10
PROTEGRIN	RGGRLCYCRRRFCVCVGR	18
SA-CATH	KFFKKLKKSVKKHVKKFFKKPKVIGVSIPF	30
SAAP-148	LKRVWKRVFKLLKRYWRQLKKPVR	24
SMAP-29-APD	RGLRRLGRKIAHGVKKYGPTVLIIRIAG	29
TACHYPLESIN	KWCFRVCYRGICYRKCR	17
TEMPORIN-1OLA	FLPFLKSILGKIL	13

**Table S15.** Peptide List for our Positive Dataset (Cont.)

Name	Seq	Seq Length
TEMPORIN-B	LLPIVGNLKSLL	13
TEMPORIN-1CEB	ILPILSLLIGGLLGK	14
TEMPORIN-GHC	FLQHIIGALTHIF	13
TEMPORIN-GHD	FLQHIIGALSHFF	13
TEMPORIN-PTA	FFGSVILKLIPKIL	13
TETRAF2W-RK	WWWLRKIW	8
TOAP1	FIGMIPGLIGGLISAFK	17
TOAP2	FFGTLFKLGSKLIPGVMKLFSSKKER	26
TSAP-2	FLGMIPGLIGGLISAFK	17
UYCT3	ILSAIWSGIKSLF	13
VLL-28	VLLVTLTRLHQRGVIYRKWRHFSGRKYR	28
ZMD32	RTCQSQSFRGPCLRRSNANCRTEGFPGGRCRGFRRRCFTTHC	47
BMAP-27	GRFKRFRKKFKLFLSPVILLHL	26
BMAP-28	GGLRSLGRKILRAWKKYGPPIVPIRI	27
SMAP-29	RGLRRLGRKIAHGVKKYGPTVLRIIRIA	28
KSL	KKVVFKVFKF	10
F2-5-12W	RWGRWLRKIRRWRPK	15
LL-31	LLGDFFRKSKEIGKEFKRIVQRIKDFLRNL	31
LL7-31	RKSKEIGKEFKRIVQRIKDFLRNL	25
LL13-37	IGKEFKRIVQRIKDFLRNLVPRTES	25
LL7-37	RKSKEIGKEFKRIVQRIKDFLRNLVPRTES	31
LL-19	LLGDFFRKSKEIGKEFKR	19
LL-25	LLGDFFRKSKEIGKEFKRIVQRIK	25
LL-13	LLGDFFRKSKEKI	13
LL13-31	IGKEFKRIVQRIKDFLRNL	19
LL7-25	RKSKEIGKEFKRIVQRIK	19
LL13-25	IGKEFKRIVQRIK	13
LL19-37	RIVQRIKDFLRNLVPRTES	19
KSL-W	KKVVFVWKFK	10
KS-30	KSKEKIGKEFKRIVQRIKDFLRNLVPRTES	30
KR-20	KRIVQRIKDFLRNLVPRTES	20
KR-12	KRIVQRIKDFLR	12
LACTOFERRICIN-(17-30)	FKCRRWQWRMKKLG	14
LACTOFERRAMPIN	WKLLSKAQEKFGKNKSR	17
MUC7-12-MER-L	RKSYKCLHKRCR	12
G10KHC	KKHRKHRKHRKGSGGSKNLRIIRKGHIKKY	36
MUC7-12-MER-L4	RKSYKALHKRAR	12
MUC7-20-MER	LAHQKPFIRKSYKCLHKRCR	20
HSN5	AKRHGYKRKFH	12
MAGAININ-II	GIGKFLHSACKFGKAFVGEIMNS	23
LYS-A1	KIFGAIWPLALGALKNLIK	19
AAP2	FHFFHHFFFHHF	14
CSP	SGSLSTFFRLFNRSFTQALGK	21
CSPC16	TFFRLFNRSFTQALGK	16
G2	KNLRIIRKGHIKKY	16
C16G2	TFFRLFNRSFTQALGKGGGKNLRIIRKGHIKKY	35
M8G2	TFFRLFNRRGGGKNLRIIRKGHIKKY	27
S6L3-33	FKKFWKWFRRF	11
C16-33	TRRRLFNRSFTQALGKSGGGFKFWKWFRRF	31
M8-33	TFFRLFNRSGGGFKFWKWFRRF	23
CECROPIN-A-(1-7)-MELITTIN	KWKLFKKIGAVLKVL	15
HH15	KRFRIRVRVIRK	12

**Table S16.** Peptide List for our Positive Dataset (Cont.)

Name	Seq	Seq Length
BAC2A	RLARIVVIRVAR	12
1026	VQWRIRVRVIKK	12
1029	KQFRIRRV	9
1036	VQFRIRVRIVIRK	13
1037	KRFRIRRV	9
HH2	VQLRIRVAVIRA	12
1002	VQRWLIVWRIRK	12
1003	IVWKIKRWWVGR	12
1004	RFWKVVRVKYIRF	12
1008	RIKWIVRFR	9
HH7	VRLRIRVAVRRA	12
1010	IRWRIRVVVRRI	12
1011	RRWVVWRIVQRR	12
1012	IFWRRIVIVKKF	12
1013	VRLRIRVA	8
1016	LRIRWIFKR	9
HH8	VRLRIRVAVIRK	12
1020	VRLRIRWWVLRK	12
HH10	KRFRIRVAVRRA	12
1035	KRWRWIVRNIRR	12
1031	WRWRVWRVWR	9
IMB-2	TFFRLFNRGGGWGSFFKAAHVGKL	25
BAC8C	RIWVIWRR	8
PTP-7	FLGALFKALSKLL	13
HOLOTHURIOIDIN-1	HLGHHALDHLLK	12
HOLOTHURIOIDIN-2	ASHLGHHALDHLLK	14
TN-AFP1	LMCTHPLDCSN	11
COPRISIN-BAAMP	VTCDVLSFEAKGIAVNH	17
HISTATIN	DSHAKRHGYKRKFHEKHHSHRGY	24
HST	AKRHHGYKRKFHG	15
DF17-6K	KKKKKKAAFAAAWAFAA	17
DF21-10K	KKKKKKKKKAFAAAWAFAA	21
CWR11	CWFWKWWRRRR	12
CHRYSTOPHSIN-1	FFGWLIKGAIHAGKAIHGLIHR	25
RK1	RWKRWWRKK	10
RK2	RKKRWWRKK	10
(IRIK)	IRIKIRIK	8
(IRVK)	IRVKIRVKIRVK	12
ALPHA-DEFENSIN-3	DCYCRIPACIAGERRYGTIYQGRLWAFCC	30
BETA-DEFENSIN-1	DHYNCVSSGGQCLYSACPIFTKIQGTCYRGKAKCCK	36
MAGAININ-I	GIGKFLHSAGKFGKAFVGEIMKS	23
RIP	YSPWTNF	7
K4-S4(1~13)A	ALWKTLLKKVLKA	13
DD13-RIP	ALWKTLLKKVLKAYSPWTNF	20
2C-4	RWRWRWF	7
SM6(L1)2C	FIKHFIIHRFGGGRWRWRWF	19
SM6(L3)2C	FIKHFIIRFSATRWRWRWF	19
SM6(L1)B33	FIKHFIIHRFGGGFKFWKWFRRF	23
NRC-16	GWKKWLRKGAKHLGQAAIK	19
GK7	GQIINLK	7
(RW)2-NH2	RWRW	4
(RW)3-NH2	RWRWRW	6

**Table S17.** Peptide List for our Positive Dataset (Cont.)

Name	Seq	Seq Length
(RW)4-NH2	RWRWRWRW	8
LASIO-III	VNWKKILGKIIKVVK	15
MELITTIN	GIGAVLKVLTTGLPALISWIKRKRQQ	26
MELIMINE	TLISWIKNKRQQRPRVSRRRRRGGRRRR	29
MELIMINE-CYSN	CTLISWIKNKRQQRPRVSRRRRRGGRRRR	30
MELIMINE-CYSC	TLISWIKNKRQQRPRVSRRRRRGGRRRRC	30
MELIMINE-CYS13	TLISWIKNKRQQRPRVSRRRRRGGRRRR	30
K4-S4(1-15)A	LWKTLKKVLKAAA	14
BETA6-20-G3K6	NEEGFFSARGHRPLDGGGKKKKKK	24
HEPCIDIN	ICIFCCGCCRSKCGMCCKT	20
NA-CATH-BAAMP	KRFKKFFKKLKNVKRAKKFFKKPKVIGVTFPF	34
NA-CATH-ATRA1-ATRA1	KRFKKFFKKLKNVKRFKKFKKLKVIGVTFPF	34
LACTOFERRICIN-B-(17-41)	FKCRRWQWRMKKLGAPSITCVRRAF	25
SCRAMBLED	GLKLRFEEFSKIKGEFLKTPEVRFRDIKLKDNRISVQR	37
R-FV-I16	RFRRRLFRIRVRLKKI	16
FV7	FRIRVRV	7
VSL2	AFKAFWKFKVFKVFK	13
VS2	KWFWKFKVFKVFK	11
L-K6	IKKILSKIKKLLK	13
HLF1-11	GRRRRSVQWCA	11
FS3	YAPWTNF	7
TET-213	KRWWKWWRRC	10
1010CYS	IRWRIRVVWRRIC	13
TET-20	KRWRIRVVRVIRKC	13
TET-26	WIVVIWRRKRRRC	13
FS8	YAPWTNA	7
CHROMOFUNGIN	RILSILRHQNLLKELQDLAL	20
CECROPIN-B	KWKVFKKIEKMGRNIRNGIVKAGPAIAVLGEAKAL	35
MAGAININ	GIGLFLHSAGLFLAFVGEMKS	23
CYSLASIO-III	CVNWKKILGKIIKVVK	16
DASAMP1	FFGKVLKLIRKIF	13
BMAP-18	GRWKWRKKWKKLWKKLS	18
BACTENECIN	RLCRIVVIRVCR	12
CA-MA	KWKLFKKIGIGKFLHSAKKF	20
RTA3	RPAFRKAAFRVMRACV	16
DHVAR5	LLLFLLKKRKKRKY	14
KABT-AMP	GIWKKWIKKWLKLLKKLWKKG	22
P10	LAREYKKIVEKLKRWLRLQVLRTL	24
P60.4AC	IGKEFKRIVERIKRFLRELVRPLR	24
OSIP108	MLCVLQGLRE	10
S-OSIP108	ELRLVCMGQL	10
[CYC2]OSIP108	MLCVLQGLREGG	12
[CYC3]OSIP108	MLCVLQGLREC	11
1018	VRLIVAVRIWRR	12
HE1	RRWIRVAVILRV	12
HE2	VRLIRAVRAWRV	12
HE3	VRWARVARILRV	12
HE4	VRLIWAVRIWRR	12
HE10	VRLIVAVRIWRR	10
HE12	RFKRVARVIW	10
GL13KR1	IGIKLLKSKLKAL	13
(IKIK)2	IKIKIKIK	8

**Table S18.** Peptide List for our Positive Dataset (Cont.)

Name	Seq	Seq Length
RI1012	FKKVIVIRRWF	12
RI1002	KRIRWVILWRQV	12
LJK1	VFLRRIRVIVIR	12
RIJK1	RIVIVRIRRLFV	12
LJK2	VFWRRIRVVWIR	12
RIJK2	RIVWVRIRRWVF	12
LJK3	VQLRAIRVRVIR	12
RIJK3	RIVRVRIARLQV	12
LJK4	VQLRRIRVWVIR	12
RIJK4	RIVWVRIRRLQV	12
LJK5	VQWRAIRVRVIR	12
RIJK5	RIVRVRAIRWQV	12
LJK6	VQWRRIRVWVIR	12
RIJK6	RIVWVRIRRWQV	12
NAL-P-113	AKRRRGYKRKFKK	13
P15	GTPGPQGIAGQRGVV	15
P15-CSP	GTPGPQGIAGQRGVVAEEAAKEAAAKEYAKASGSLSTFFRLFNRSFTQALGK	53
C-GG-NT-DHVAR5	CGGLLFLKKRKKRKY	17
KT2	NGVQPKYKWWKWWKKWW	17
RT2	NGVQPKYRWWWRWWRRWW	17
LF11-322	PFWRIRIRR	9
LF11-324	PFFWRIRIRR	10
6-MO-LF11-227	FWRRFWRR	8
LF11-215	FWRIRIRR	8
D-ATRA-1A	KRAKKFFKKLK	11
ATRA-2	KRAKKFFKKPK	11
ATRA-1	KRFKKFFKKLK	11
ALL	LKLLKKLLKKLLKLL	15
SEG5D	KKLLLLLLLLKKKK	15
SEG6D	LLLLLKKKKKKL	15
G10	KNLRRRIRKGIHIKKYG	18
LIN-SB056	WKKIRVRLSA	10
LIN-SB056-1	KWKIRVRLSA	10
MYXINIDIN2	KIKWILKYWKWS	12
MYXINIDIN3	RIRWILRYWRWS	12
GH12	GLLWHLLLHHLLLH	12
PA-MAP	LAAKLTKAATKLTAALTKLAAALT	24
HSAFP1	DGVKLCDVPSGTWSGHCGSSSKCSQQCKDREHFAYGGACHYQFPSVKCFCKRQC	54
HSLIN06	EHFAYGGAKHYQFPSVKFKKRQK	24
Verine	RRRWWWWV	8
Phylloseptin-PTa	FLSLIPKIAGGIAALAKHL	19

## 7.2 MBEC Dataset

Antibiofilm peptides with MBEC values are listed in Tables S19–S20. The pathogens against which the MBEC values are effective are also listed in the ‘pathogen’ column. The MBEC values are listed in  $\mu\text{M}$ .

**Table S19.** Antibiofilm Peptides and MBEC ( $\mu\text{M}$ ) Values

Name	Seq	MBEC ( $\mu\text{M}$ )	Pathogen	Source
BREVININ-1GHA	FLGAVLKAGKLVPAACKISKKC	16	<i>S. aureus</i>	Chen et al. (2018)
DERMASEPTIN-AC4	SLWGKLKEMAAAAGKAALNAVGLVNQ	256	<i>S. aureus</i>	Gong et al. (2020)
KASSINIATUERIN-3	FIQHLIPLIPHAIQGQIKDIF	64	<i>S. aureus</i>	Wang et al. (2020)
CCL20	SNFDCCCLGYTDRLHPKFIVGFTRQLANECDINAIIFH TKKKL SVCANPKQTWVKYIVRLLSKKVKNM	128	<i>P. aeruginosa</i>	Ramamourthy et al. (2019)
COPRISIN	VTCDVLSFEAKGIAVNHSACALHCIALRKKGSCQNG VCVCRN	4.49	<i>P. aeruginosa</i>	Hwang et al. (2013)
DERMASEPTIN-PH	ALWKEVLKNAGKAALNEINNLV	128	<i>S. aureus</i>	Huang et al. (2017)
DERMASEPTIN-PT9	GLWSKIKDAAKTAGKAALGFVNEMV	32	<i>S. aureus</i>	Li et al. (2019)
ESCULENTIN	GIFS KLAGKKIKNLISGLKG	6	<i>P. aeruginosa</i>	Luca et al. (2013)
GL13K	GKIIKLKASLKL	22.47	<i>P. aeruginosa</i>	Hirt and Gorr (2013)
HUMAN defensin	GIINTLQKYCRVRRGGRCAVLSCLPKEEQIGKCSTRGR KCCRRKK	3.1	MRSE	Sutton and Pritts (2014)
INDOLICIDIN	ILPWKWPWWPWR	335.7	MRSA	Mataraci and Dosler (2012)
LL-37	LLGDFFRKSKEKIGKEFKRIVQRIKDFRLRNLPRTES	20	<i>P. aeruginosa</i>	Nagant et al. (2012)
NISIN	ITSISLCTPGCKTGALMGNCNMKTATCHCSIHVSK	183.1	MRSA	Mataraci and Dosler (2012)
PHYLLOSEPTIN-1	FLSLIPHIVSGVASIAKH	5	<i>S. aureus</i>	Zhang et al. (2010)
PLEUROCIDIN	GWGSFFKKAAHVGVKHVGKAALTHYL	23.62	<i>S. mutans</i>	Tao et al. (2011)
BMAP-27	GRFKRFFKKFKLKKLSPVIPLLHL	6.2	<i>P. aeruginosa</i>	Pompilio et al. (2011)
BMAP-28	GGRLSLGRKILRAWKKYGPPIVPIIRI	6.5	<i>P. aeruginosa</i>	Pompilio et al. (2011)
SMAP-29	RGLRLRKRKIAHVVKYGPVLRRIIA	6.25	<i>P. aeruginosa</i>	Pompilio et al. (2011)
KSL	KKVVFVKVFK	400	<i>S. mutans</i>	Liu et al. (2011)
F2-5-12W	RWGRWLKRIRRWRPK	40	<i>S. epidermidis</i>	Molhoek et al. (2011)
LL-31	LLGDFFRKSKEKIGKEFKRIVQRIKDFRLN	20	<i>P. aeruginosa</i>	Nagant et al. (2012)
LL13-37	IGKEFKRIVQRIKDFRLRNLPRTES	100	<i>P. aeruginosa</i>	Nagant et al. (2012)
LL7-37	RKSKEKIGKEFKRIVQRIKDFRLRNLPRTES	50	<i>P. aeruginosa</i>	Nagant et al. (2012)
KSL-W	KKVVFWVKFK	191.16	MRSA	Gawande et al. (2014)
MUC7-12-MER-L	RKS YKCLHKR CR	12.5→50; median 50	<i>S. mutans</i>	Wei et al. (2006)
MUC7-12-MER-L4	RKS YKALHKR AR	50; median >50	<i>S. mutans</i>	Wei et al. (2006)
MUC7-20-MER	LAHQKPFIRKS YKCLHKR CR	6.25→25; median 25	<i>S. mutans</i>	Wei et al. (2006)
HSN5	AKRHHGYKRKFH	12.5→50; median >50	<i>S. mutans</i>	Wei et al. (2006)
MAGAININ-II	GIGKFLHSACKFGKAFVGEIMNS	25→50; median >50	<i>S. mutans</i>	Wei et al. (2006)
C16G2	TF FRLFNRSFTQALGKGGGKNLRIIRKGHIKKY	25	<i>S. mutans</i>	Sullivan et al. (2011)
BAC8C	RIWVIWRR	108.13	<i>S. mutans</i>	Ding et al. (2014)
PTP-7	FLGALFKALSKLL	40	<i>S. aureus</i>	Kharidia and Liang (2011)
CHRYSOPHSIN-1	FFGWLKGAIHAGKAIHGLIHRHH	11.07	<i>S. aureus</i>	Wang et al. (2012)
2C-4	RWRWRWF	50	<i>S. mutans</i> and other oral streptococci	He et al. (2010)
SM6(L1)2C	FIKHF IHRFGGGF KKFWKWF RRF	50	<i>S. mutans</i> and other oral streptococci	He et al. (2010)
SM6(L3)2C	FIKHF IHRFSATRWRWRWF	50	<i>S. mutans</i> and other oral streptococci	He et al. (2010)
SM6(L1)B33	FIKHF IHRFGGGF KKFWKWF RRF	50	<i>S. mutans</i>	He et al. (2010)
(RW)4-NH2	RWRWRWRW	100	<i>E. coli</i>	Hou et al. (2010)
MELITTIN	GIGAVLKVLTTGLPALISWIKRKRQQ	50	<i>S. mutans</i>	Sullivan et al. (2011)
R-FV-I16	RFRRRLFIRVRVLKKI	64	<i>P. aeruginosa</i>	Xu et al. (2014)
L-K6	IKKILSKIKKLLK	6.25	<i>S. mutans</i>	Shang et al. (2014)
CA-MA	KWKLFKKIGIGKFLHSACKF	361.54	MRSA	Mataraci and Dosler (2012)
P10	LAREYKKIVEKLKRWLRQLRTL	32	MRSA	Haisma et al. (2014)

**Table S20.** Antibiofilm Peptides and MBEC ( $\mu\text{M}$ ) Values (Cont...)

Name	Seq	MBEC ( $\mu\text{M}$ )	Pathogen	Source
1018	VRLIVAVRIWRR	6.51	<i>P. aeruginosa</i>	<a href="#">de la Fuente-Núñez et al. (2013)</a>
HE4	VRLIWAVRIWRR	6.16	<i>P. aeruginosa</i>	<a href="#">de la Fuente-Núñez et al. (2014)</a>
HE10	VRLIVRIWRR	7.32	<i>P. aeruginosa</i>	<a href="#">de la Fuente-Núñez et al. (2014)</a>
DJK5	VQWRAIRVRVIR	1.61	<i>P. aeruginosa</i>	<a href="#">de la Fuente-Núñez et al. (2015)</a>
DJK6	VQWRRIRVWVIR	1.5	<i>P. aeruginosa</i>	<a href="#">de la Fuente-Núñez et al. (2015)</a>
KT2	NGVQPKYKWWKWWKKWW	1	<i>E. coli</i>	<a href="#">Anunthawan et al. (2015)</a>
RT2	NGVQPKYRWWWRWWRRWW	1	<i>E. coli</i>	<a href="#">Anunthawan et al. (2015)</a>
DI-MB-LF11-322	PFWRIRIRR	246.38	<i>P. aeruginosa</i>	<a href="#">Sánchez-Gómez et al. (2015)</a>
LF11-324	PFFWRIRIRR	55.33	<i>P. aeruginosa</i>	<a href="#">Sánchez-Gómez et al. (2015)</a>
6-MO-LF11-227	FWRRFWRR	489.01	<i>P. aeruginosa</i>	<a href="#">Sánchez-Gómez et al. (2015)</a>
LF11-215	FWRIRIRR	133.41	<i>P. aeruginosa</i>	<a href="#">Sánchez-Gómez et al. (2015)</a>
P60.4AC	IGKEFKRIVERIKRFLRELVRPLR	32	MRSA	<a href="#">Haisma et al. (2014)</a>

## REFERENCES

- Anunthawan, T., de la Fuente-Núñez, C., Hancock, R. E., and Klaynongsruang, S. (2015). Cationic amphipathic peptides kt2 and rt2 are taken up into bacterial cells and kill planktonic and biofilm bacteria. *Biochimica et Biophysica Acta (BBA) - Biomembranes* 1848, 1352–1358. doi:<https://doi.org/10.1016/j.bbamem.2015.02.021>
- [Dataset] Armstrong, D. and Zidovetzki, R. (2009). Helical wheel projections. [www.donarmstrong.com/cgi-bin/wheel.pl](http://www.donarmstrong.com/cgi-bin/wheel.pl). Version ID: wheel.pl,v 1.4 2009-10-20 21:23:36 don Exp
- Chen, Q., Cheng, P., Ma, C., Xi, X., Wang, L., Zhou, M., et al. (2018). Evaluating the bioactivity of a novel broad-spectrum antimicrobial peptide brevinin-1gha from the frog skin secretion of hylarana guentheri and its analogues. *Toxins* 10. doi:10.3390/toxins10100413
- de la Fuente-Núñez, C., Mansour, S. C., Wang, Z., Jiang, L., Breidenstein, E. B., Elliott, M., et al. (2014). Anti-biofilm and immunomodulatory activities of peptides that inhibit biofilms formed by pathogens isolated from cystic fibrosis patients. *Antibiotics* 3, 509–526. doi:10.3390/antibiotics3040509
- de la Fuente-Núñez, C., Reffuveille, F., Mansour, S. C., Reckseidler-Zenteno, S. L., Hernández, D., Brackman, G., et al. (2015). D-enantiomeric peptides that eradicate wild-type and multidrug-resistant biofilms and protect against lethal *Pseudomonas aeruginosa* infections. *Chem Biol* 22, 196–205
- de la Fuente-Núñez, C., Reffuveille, F., nde, L. F., and Hancock, R. E. (2013). Bacterial biofilm development as a multicellular adaptation: antibiotic resistance and new therapeutic strategies. *Current Opinion in Microbiology* 16, 580–589. doi:10.1016/j.mib.2013.06.013. Antimicrobials · Genomics
- Ding, Y., Wang, W., Fan, M., Tong, Z., Kuang, R., Jiang, W., et al. (2014). Antimicrobial and anti-biofilm effect of Bac8c on major bacteria associated with dental caries and *Streptococcus mutans* biofilms. *Peptides* 52, 61–67
- Gawande, P. V., Leung, K. P., and Madhyastha, S. (2014). Antibiofilm and antimicrobial efficacy of dispersinB®-ksl-w peptide-based wound gel against chronic wound infection associated bacteria. *Current Microbiology* 68, 635–641. doi:10.1007/s00284-014-0519-6
- Gong, Z., Pei, X., Ren, S., Chen, X., Wang, L., Ma, C., et al. (2020). Identification and rational design of a novel antibacterial peptide dermaseptin-ac from the skin secretion of the red-eyed tree frog agalychnis callidryas. *Antibiotics* 9. doi:10.3390/antibiotics9050243
- Gupta, S., Sharma, A. K., Jaiswal, S. K., and Sharma, V. K. (2016). Prediction of biofilm inhibiting peptides: An in silico approach. *Frontiers in Microbiology* 7, 949. doi:10.3389/fmicb.2016.00949
- Haisma, E. M., de Breij, A., Chan, H., van Dissel, J. T., Drijfhout, J. W., Hiemstra, P. S., et al. (2014). LL-37-derived peptides eradicate multidrug-resistant *staphylococcus aureus* from thermally wounded human skin equivalents. *Antimicrobial Agents and Chemotherapy* 58, 4411–4419. doi:10.1128/AAC.02554-14

- He, J., Yarbrough, D. K., Kreth, J., Anderson, M. H., Shi, W., and Eckert, R. (2010). Systematic approach to optimizing specifically targeted antimicrobial peptides against *streptococcus mutans*. *Antimicrobial Agents and Chemotherapy* 54, 2143–2151. doi:10.1128/AAC.01391-09
- Hirt, H. and Gorr, S.-U. (2013). Antimicrobial peptide gl13k is effective in reducing biofilms of *pseudomonas aeruginosa*. *Antimicrobial Agents and Chemotherapy* 57, 4903–4910. doi:10.1128/AAC.00311-13
- Hou, S., Liu, Z., Young, A. W., Mark, S. L., Kallenbach, N. R., and Ren, D. (2010). Effects of trp- and arg-containing antimicrobial-peptide structure on inhibition of *escherichia coli* planktonic growth and biofilm formation. *Applied and Environmental Microbiology* 76, 1967–1974. doi:10.1128/AEM.02321-09
- Huang, L., Chen, D., Wang, L., Lin, C., Ma, C., Xi, X., et al. (2017). Dermaseptin-ph: A novel peptide with antimicrobial and anticancer activities from the skin secretion of the south american orange-legged leaf frog, pithecopus (phyllomedusa) hypochondrialis. *Molecules* 22. doi:10.3390/molecules22101805
- Hwang, I.-s., Hwang, J.-S., Hwang, J. H., Choi, H., Lee, E., Kim, Y., et al. (2013). Synergistic effect and antibiofilm activity between the antimicrobial peptide coprisin and conventional antibiotics against opportunistic bacteria. *Current Microbiology* 66, 56–60. doi:10.1007/s00284-012-0239-8
- Kharidia, R. and Liang, J. F. (2011). The activity of a small lytic peptide PTP-7 on *Staphylococcus aureus* biofilms. *J Microbiol* 49, 663–668
- Li, M., Xi, X., Ma, C., Chen, X., Zhou, M., Burrows, J. F., et al. (2019). A novel dermaseptin isolated from the skin secretion of phyllomedusa tarsius and its cationicity-enhanced analogue exhibiting effective antimicrobial and anti-proliferative activities. *Biomolecules* 9. doi:10.3390/biom9100628
- Liu, Y., Wang, L., Zhou, X., Hu, S., Zhang, S., and Wu, H. (2011). Effect of the antimicrobial decapeptide KSL on the growth of oral pathogens and *Streptococcus mutans* biofilm. *Int J Antimicrob Agents* 37, 33–38
- Luca, V., Stringaro, A., Colone, M., Pini, A., and Mangoni, M. L. (2013). Esculentin(1-21), an amphibian skin membrane-active peptide with potent activity on both planktonic and biofilm cells of the bacterial pathogen *pseudomonas aeruginosa*. *Cellular and Molecular Life Sciences* 70, 2773–2786. doi:10.1007/s00018-013-1291-7
- Madeira, F., Park, Y. M., Lee, J., Buso, N., Gur, T., Madhusoodanan, N., et al. (2019). The embl-ebi search and sequence analysis tools apis in 2019. *Nucleic acids research* 47, W636—W641. doi:10.1093/nar/gkz268
- Mataraci, E. and Dosler, S. (2012). In vitro activities of antibiotics and antimicrobial cationic peptides alone and in combination against methicillin-resistant *Staphylococcus aureus* biofilms. *Antimicrob Agents Chemother* 56, 6366–6371
- Molhoek, E. M., van Dijk, A., Veldhuizen, E. J., Haagsman, H. P., and Bikker, F. J. (2011). A cathelicidin-2-derived peptide effectively impairs *Staphylococcus epidermidis* biofilms. *Int J Antimicrob Agents* 37, 476–479
- Nagant, C., Pitts, B., Nazmi, K., Vandenbranden, M., Bolscher, J. G., Stewart, P. S., et al. (2012). Identification of peptides derived from the human antimicrobial peptide ll-37 active against biofilms formed by *pseudomonas aeruginosa* using a library of truncated fragments. *Antimicrobial Agents and Chemotherapy* 56, 5698–5708. doi:10.1128/AAC.00918-12
- Pompilio, A., Scocchi, M., Pomponio, S., Guida, F., Di Primio, A., Ficarelli, E., et al. (2011). Antibacterial and anti-biofilm effects of cathelicidin peptides against pathogens isolated from cystic fibrosis patients. *Peptides* 32, 1807–1814

- Ramamourthy, G., Arias, M., Nguyen, L. T., Ishida, H., and Vogel, H. J. (2019). Expression and purification of chemokine mip-3 $\alpha$  (ccl20) through a calmodulin-fusion protein system. *Microorganisms* 7. doi:10.3390/microorganisms7010008
- Sánchez-Gómez, S., Ferrer-Espada, R., Stewart, P. S., Pitts, B., Lohner, K., and Martínez de Tejada, G. (2015). Antimicrobial activity of synthetic cationic peptides and lipopeptides derived from human lactoferricin against *pseudomonas aeruginosa* planktonic cultures and biofilms. *BMC Microbiology* 15, 137. doi:10.1186/s12866-015-0473-x
- Schiffer, M. and Edmundson, A. B. (1967). Use of helical wheels to represent the structures of proteins and to identify segments with helical potential. *Biophysical journal* 7, 121–135. doi:10.1016/S0006-3495(67)86579-2
- Shang, D., Liang, H., Wei, S., Yan, X., Yang, Q., and Sun, Y. (2014). Effects of antimicrobial peptide L-K6, a temporin-1CEb analog on oral pathogen growth, *Streptococcus mutans* biofilm formation, and anti-inflammatory activity. *Appl Microbiol Biotechnol* 98, 8685–8695
- Singh, H., Singh, S., and Singh Raghava, G. P. (2019). Peptide secondary structure prediction using evolutionary information. *bioRxiv* doi:10.1101/558791
- Sullivan, R., Santarpia, P., Lavender, S., Gittins, E., Liu, Z., Anderson, M. H., et al. (2011). Clinical efficacy of a specifically targeted antimicrobial peptide mouth rinse: Targeted elimination of  $\beta$ -streptococcus mutans;  $\beta$ -defensin 3 and prevention of demineralization. *Caries Research* 45, 415–428. doi:10.1159/000330510
- Sutton, J. M. and Pritts, T. A. (2014). Human beta-defensin 3: a novel inhibitor of *Staphylococcus*-produced biofilm production. Commentary on “Human  $\beta$ -defensin 3 inhibits antibiotic-resistant *Staphylococcus* biofilm formation”. *J Surg Res* 186, 99–100
- Tao, R., Tong, Z., Lin, Y., Xue, Y., Wang, W., Kuang, R., et al. (2011). Antimicrobial and antibiofilm activity of pleurocidin against cariogenic microorganisms. *Peptides* 32, 1748–1754
- Wang, H., He, H., Chen, X., Zhou, M., Wei, M., Xi, X., et al. (2020). A novel antimicrobial peptide (kassinatuerin-3) isolated from the skin secretion of the african frog, *kassina senegalensis*. *Biology (Basel)* 9
- Wang, W., Tao, R., Tong, Z., Ding, Y., Kuang, R., Zhai, S., et al. (2012). Effect of a novel antimicrobial peptide chrysophsin-1 on oral pathogens and *Streptococcus mutans* biofilms. *Peptides* 33, 212–219
- Waterhouse, A. M., Procter, J. B., Martin, D. M. A., Clamp, M., and Barton, G. J. (2009). Jalview version 2—a multiple sequence alignment editor and analysis workbench. *Bioinformatics* 25, 1189–1191. doi:10.1093/bioinformatics/btp033
- Wei, G.-X., Campagna, A. N., and Bobek, L. A. (2006). Effect of muc7 peptides on the growth of bacteria and on *streptococcus mutans* biofilm. *Journal of Antimicrobial Chemotherapy* 57, 1100–1109. doi:10.1093/jac/dkl120
- Xu, W., Zhu, X., Tan, T., Li, W., and Shan, A. (2014). Design of embedded-hybrid antimicrobial peptides with enhanced cell selectivity and anti-biofilm activity. *PLOS ONE* 9, 1–13. doi:10.1371/journal.pone.0098935
- Zhang, R., Zhou, M., Wang, L., McGrath, S., Chen, T., Chen, X., et al. (2010). Phylloseptin-1 (psn-1) from phyllomedusa sauvagei skin secretion: a novel broad-spectrum antimicrobial peptide with antibiofilm activity. *Molecular Immunology* 47 11-12, 2030–7